

55 56 57 61 62 64 65 66 67 68 69 80 84 85 86 87 88 91 92 93 ring nodes : 1 2 3 4 5 6 17 18 19 20 21 22 71 72 73 74 75 76 77 78 79 chain bonds : 7-8 7-84 7-91 8-36 8-92 10-61 10-11 10-92 11-12 11-64 11-65 12-14 14-15 14-62 15-16 15-48 16-18 30-31 37-38 39-40 50-51 54-55 56-57 66-67 66-68 66-69 79-80 85-87 85-88 85-86 92-93 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76 72-73 73-74 74-75 75-76 75-77 76-79 77-78 78-79 exact/norm bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-84 7-91 8-36 10-61 10-11 11-12 11-64 11-65 12-14 14-15 14-62 15-48 30-31 54-55 56-57 76-79 78-79 92-93 exact bonds : 7-8 8-92 10-92 15-16 16-18 37-38 39-40 50-51 66-67 66-68 66-69 75-77 77-78 79-80 85-87 85-88 85-86 normalized bonds : 17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76 72-73 73-74 74-75 75-76 isolated ring systems : containing 1 : 17 : 71 :

7 8 10 11 12 14 15 16 26 30 31 33 36 37 38 39 40 44 48 49

50 51 54

G2:CH3,Et

G1:0,S

G5:Ak,H,OH,[*1]

G4:CH3,Et,H

chain nodes :

G6:Ak,Cb,[*2],[*3]

```
G7:COOH, Ak, H, [*4]
```

G8: [*5], [*6], [*7], [*8]

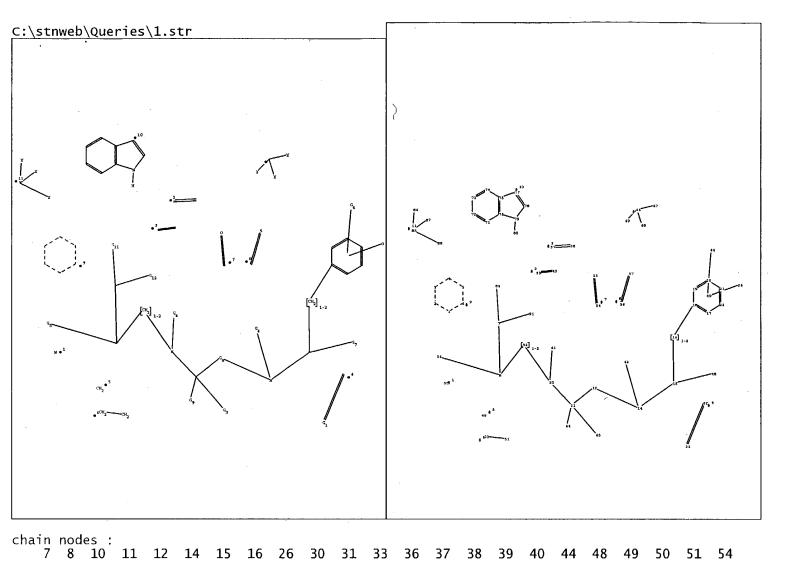
G9:Ak,Ph

G11:[*9],[*10]

G12:H,OH,NH2,CN,[*11]

```
Match level:
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 26:CLASS 27:CLASS 30:CLASS 31:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 44:CLASS 45:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 54:CLASS 54:CLASS 62:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 55:CLASS 56:CLASS 57:CLASS 61:CLASS 73:Atom 74:Atom 75:Atom 76:Atom 77:CLASS 69:CLASS 71:CLASS 72:CLASS 68:CLASS 78:CLASS 79:CLASS 80:CLASS 84:CLASS 85:CLASS 86:CLASS 87:CLASS 88:CLASS 91:CLASS 92:CLASS 93:CLASS



55 56 57 61 62 64 65 66 67 68 69 80 84 85 86 87 88 91 92 1 2 3 4 5 6 17 18 19 20 21 22 71 72 73 74 75 76 77 78 79 chain bonds : 7-8 7-84 7-91 8-36 8-92 10-61 10-11 10-92 11-12 11-64 11-65 12-14 14-15 14-62 15-16 15-48 16-18 30-31 37-38 39-40 50-51 54-55 56-57 66-67 66-68 66-69 79-80 85-87 85-88 85-86 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76 72-73 73-74 74-75 75-76 75-77 76-79 77-78 78-79 exact/norm bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-84 7-91 8-36 10-61 10-11 11-12 11-64 11-65 12-14 14-15 14-62 15-48 30-31 54-55 56-57 76-79 78-79 exact bonds : 7-8 8-92 10-92 15-16 16-18 37-38 39-40 50-51 66-67 66-68 66-69 75-77 77-78 79-80 85-87 85-88 85-86 normalized bonds : 17-18 17-22 18-19 19-20 20-21 21-22 71-72 71-76 72-73 73-74 74-75 75-76 isolated ring systems : containing 1 : 17 : 71 :

G2:CH3,Et G3:H,Ak

G1:0,S

G4:CH3,Et,H G5:Ak,H,OH,[*1]

G6:Ak,Cb,[*2],[*3]

```
G7:COOH,Ak,H,[*4]
G8:[*5],[*6],[*7],[*8]
G9:Ak,Ph
G11:[*9],[*10]
G12:H,OH,NH2,CN,[*11]
Match level:
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 26:CLASS 27:CLASS 30:CLASS 31:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS
12:CLASS 14:CLASS 15:CLASS 16:CLASS 22:Atom 26:CLASS 27:CLASS 30:CLASS
                                                                                                           38:CLASS
                                                      48:CLASS 49:CLASS 50:CLASS 51:CLASS
39:CLASS
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                                                                                                            54:CLASS
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                           57:CLASS
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78:CLASS
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92:CLASS
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=> s 195

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SAMPLE SCREEN SEARCH COMPLETED - 456 TO ITERATE

100.0% PROCESSED 456 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

7839 TO 10401

PROJECTED ANSWERS:

0 TO 0

L96

0 SEA SSS SAM L95

=> s 195 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: Y
FULL SEARCH INITIATED 22:40:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9898 TO ITERATE

100.0% PROCESSED 9898 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

L97 5 SEA SSS FUL L95

=> file hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 1115.24 2615.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

ENTRY SESSION

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FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10 FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 197

L98

1 L97

=> d 198, ibib abs fhitstr, 1

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full

ACCESSION NUMBER:

2000:535162 HCAPLUS

DOCUMENT NUMBER:

133:150920

TITLE:

Preparation of peptides or analogs containing

substituted phenethylamine moiety as motilin receptor

antagonists

INVENTOR(S):

Matsuoka, Hiroharu; Sato, Tsutomu; Takahashi,

Tadakatsu; Kim, Dong Ick; Jung, Kyung Yun; Park, Chan

PATENT ASSIGNEE (S):

Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE:

PCT Int. Appl., 403 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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,	MD, M	G, MK,	MN, N	ΜW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,				
	SK, S	L, TJ,	TM,	ΓR,	TT,	TZ,	UA,	ŪĠ,	US,	UΖ,	VN,	YU,	ZA,	ZW,	AM,				
	AZ, B	Y, KG,	KZ, N	ΜD,	RU,	ТJ,	$\mathbf{T}\mathbf{M}$												
RW:	GH, G	M, KE,	LS, N	ΜW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,				
	DK, E	s, FI,	FR, C	GΒ,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,				
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EP 11498	143		A1		2001	1031		EP 20	000-	9019	<u> 56</u>								
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	IE, S	I, LT,	LV, I	FI,	RO														
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Substituted phenethylamine derivs. represented by general formula (I), AΒ hydrates of the same, or pharmaceutically acceptable salts thereof [wherein Cy is a group represented by general formula Q, an optionally substituted heterocyclic group, C3-7 cycloalkyl, or phenyl; R1, R1, R1, R1

and R5 are each hydrogen, halogeno, hydroxyl, amino, trifluoromethyl or cyano, at least one of R1-R5 being halogeno, trifluoromethyl or cyano; R6 represents hydrogen, (un) substituted linear or branched C1-3 alkyl, amino, or hydroxy; R8 represents hydrogen, Me, or ethyl; R9 represents (un) substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or C2-6 alkynyl, C3-7 cycloalkyl, or (un) substituted Ph; R20 represents hydrogen, or (un) substituted linear or branched C1-3 alkyl or R9 and R20 together forms C3-7 cycloalkyl; R10 represents hydrogen, (un) substituted linear or branched C1-3 alkyl; R11 represents hydrogen or (un) substituted linear or branched C1-3 alkyl, (un) substituted carbamoyl, or carboxy; R12 represents hydroxy or linear or branched C1-4 alkoxy; R13 represents hydrogen, (un) substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or alkynyl, etc.; X, Y represents carbonyl or CH2; provisos are given.], which exhibit motilin receptor antagonism and being useful as drugs for preventing digestive tract movement or high level of blood motilin. Thus, 3-methyl-2-methylaminobutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2pyridylcarbamoyl)ethylamide (prepn. given) was condensed with Boc-Phe(4-F)-OH using CMPI in the presence of Et3N in THF under ice-cooling for 4 h followed by treatment of the product with CF3CO2H in CH2Cl2 gave 2-((2-amino-3-(4-fluorophenyl)propanoyl)-N-methylamino)-3methylbutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2pyridylcarbamoyl)ethylamide (II). II and N-Et-Phe(4-F)-N-Me-Val-N-Et-Tyr(3-tBu)-NHEt showed IC50 of 0.35 and 0.17 nM, resp., for inhibiting binding of 1251-motilin to motilin receptor prepn. from mucus membrane of rabbit duodenum.

IT 287207-09-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides or analogs contg. substituted phenethylamine moiety as motilin receptor antagonists and drugs for preventing digestive tract movement or high level of blood motilin)

RN 287207-09-4 HCAPLUS

CN L-Tyrosinamide, 4-fluoro-L-phenylalanyl-(2S)-4,4,4-trifluoro-2-(methylamino)butanoyl-3-(1,1-dimethylethyl)-N\alpha-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

7.12 2622.41

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY

TOTAL SESSION

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L4

S L4

FILE 'REGISTRY' ENTERED AT 21:28:05 ON 02 SEP 2004

L5 1 S L4

FILE 'HCAPLUS' ENTERED AT 21:28:06 ON 02 SEP 2004

L6

FILE 'REGISTRY' ENTERED AT 21:28:09 ON 02 SEP 2004

L7 STRUCTURE UPLOADED

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FILE 'HCAPLUS' ENTERED AT 21:28:41 ON 02 SEP 2004

L9 4 S L3

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L10 0 S L9

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352 S L11 FULL L13

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3 S L14 NOT L9 L15

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L97
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L98
              1 S L97
     FILE 'CAOLD' ENTERED AT 22:41:17 ON 02 SEP 2004
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0 L97

L99

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

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2622.83

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STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2 DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

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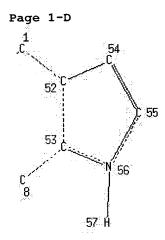
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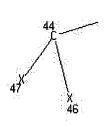
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Page 1-A 0 66 S 67

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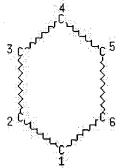
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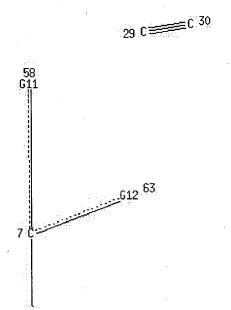
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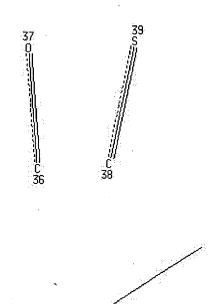
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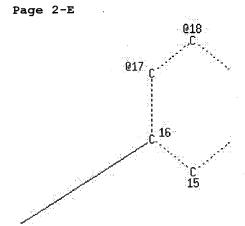




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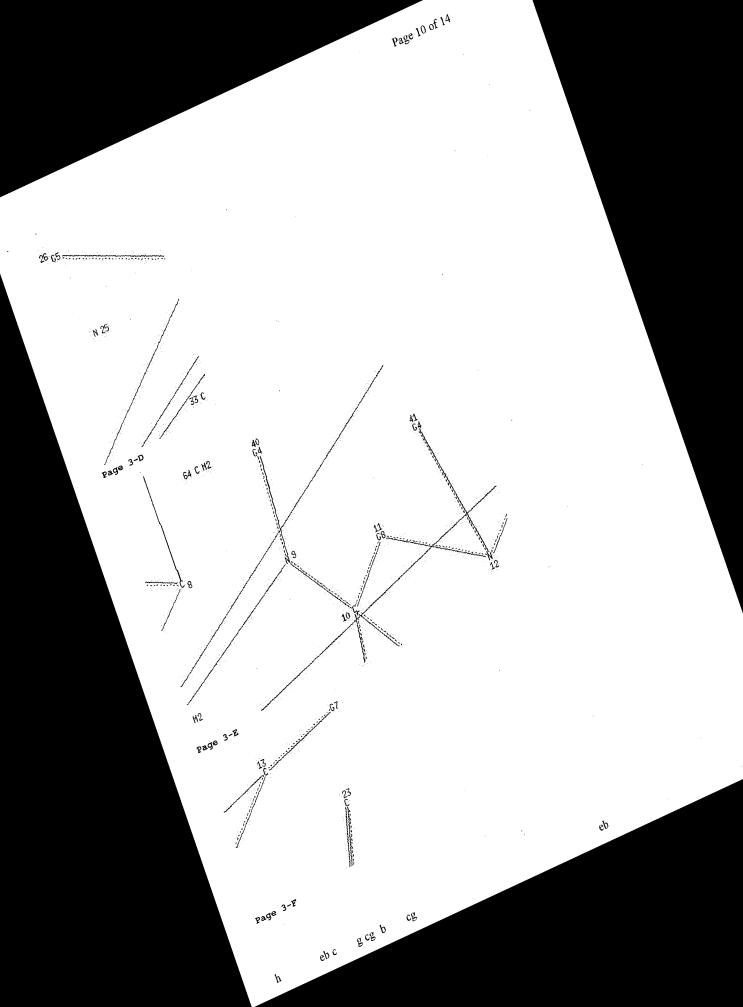


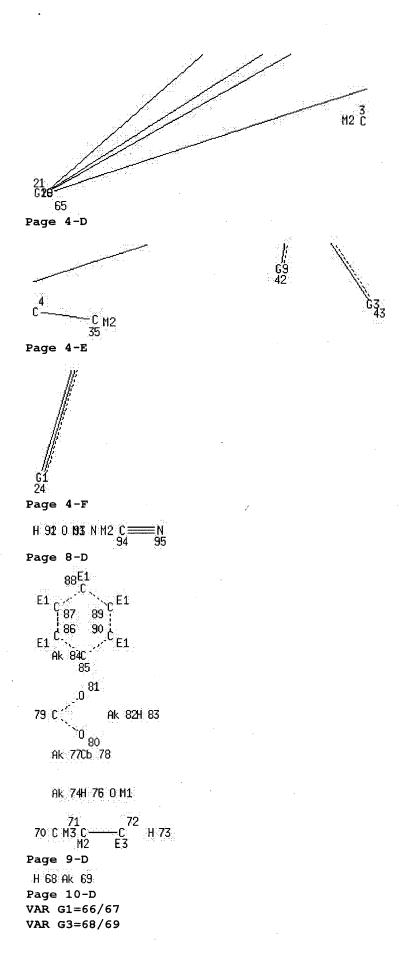




14 C M2
Page 2-F
32
Page 3-A

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VAR G5=74/75/76/25
VAR G6=77/78/27/29
VAR G7=79/82/83/23
VAR G8=33-10 33-12/34-10 34-12/36-10 36-12/38-10 38-12
VAR G9=84/85
VAR G11=6/54
VAR G12=91/92/93/94/59
REP G19=(1-2) 64-8 64-9
REP G20=(1-2) 14-13 14-16
VPA 22-18/19/20 S
VPA 31-17/18/19/20 S
NODE ATTRIBUTES:
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                    ΑT
                        14
HCOUNT
         IS M2
                    ΑT
                        33
HCOUNT
         IS M2
                    ΑT
                        34
HCOUNT
         IS M2
                    ΑT
                        35
HCOUNT
         IS M2
                    ΑT
                        64
HCOUNT
         IS M3
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                    AΤ
HCOUNT
         IS M2
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                        71
HCOUNT
        IS E3
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                        76
HCOUNT
         IS M1
                    AΤ
                    ΑT
                        86
HCOUNT
         IS E1
                        87
HCOUNT
         IS E1
                    AΤ
HCOUNT
         IS E1
                    ΑT
                        88
HCOUNT
         IS E1
                    AΤ
                        ~89
                    ΑT
HCOUNT
                        90
         IS E1
HCOUNT
         IS M1
                    ΑT
                        92
HCOUNT
         IS M2
                    AT
                        93
NSPEC
         IS R
                    AT
                         1
NSPEC
                    ΑT
         IS R
                         2
NSPEC
         IS R
                    ΑT
                         3
         IS R
NSPEC
                    AT
                         4
                         5
NSPEC
         IS R
                    ΑT
NSPEC
         IS R
                    AT
                          6
NSPEC
         IS C
                    AT
                         7
NSPEC
         IS C
                    AT
                         8
NSPEC
         IS C
                    ΑT
                         9
NSPEC
         IS C
                    ΑT
                        10
NSPEC
         IS C
                    ΑT
                        11
NSPEC
                    AT
         IS C
                        12
NSPEC
         IS C
                    AT
                        13
NSPEC
         IS C
                    AT
                        14
NSPEC
         IS R
                    AT
                        15
NSPEC
                    AT
         IS R
                        16
NSPEC
         IS R
                    ΑT
                        17
NSPEC
         IS R
                    ΑT
                        18
NSPEC
         IS R
                   AT
                        19
NSPEC
         IS R
                    AT
                        20
NSPEC
         IS C
                    AT
                        21
NSPEC
         IS C
                    ΑT
                        22
        IS C
                    AT
                        23
NSPEC
         IS C
                    AT
                        24
NSPEC
NSPEC
         IS C
                    AT,
                        25
NSPEC
         IS C
                    AT
                        26
NSPEC
         IS C
                    ΑT
                        27
NSPEC
         IS C
                    ΑT
                        28
NSPEC
         IS C
                    ΑT
                        29
         IS C
                        30
NSPEC
                    AT
NSPEC
         IS C
                    AT
                        31
```

```
IS C
                 \mathbf{AT}
                     33
NSPEC
NSPEC
        IS C
                  ΑT
                      34
NSPEC
        IS C
                  ΑT
                      35
NSPEC
        IS C
                  AΤ
                     36
NSPEC
        IS C
                  AT
                     37
NSPEC
       IS C
                  AΤ
                     38
NSPEC
      IS C
                  AΤ
                     39
       IS C
                  AT
                     40
NSPEC
       IS C
NSPEC
                  ΑT
                     41
NSPEC
        IS C
                  ΑT
                     42
NSPEC
       IS C
                  AΤ
                     43
NSPEC
      IS C
                  \mathbf{AT}
                     44
NSPEC IS C
                  AT 45
NSPEC IS C
                  \mathbf{AT}
NSPEC
       IS C
                 ΑT
                     47
NSPEC IS R
                  ΑT
                     48
NSPEC
        IS R
                  ΑT
                      49
NSPEC
        IS R
                  ΑT
                     50
NSPEC
       IS R
                 AT 51
NSPEC IS R
                 ΑT
                     52
NSPEC IS R
                 ΑT
                     53
NSPEC IS R
                 ΑT
                     54
      IS R
NSPEC
                  ΑT
                     55
      IS R
NSPEC
                  \mathbf{AT}
                      56
NSPEC
       IS C
                  AT
NSPEC IS C
                 ΑT
                     58
NSPEC IS C
                 AΤ
                     59
NSPEC IS C
                 ΑT
NSPEC IS C
                 AΤ
                      61
NSPEC IS C
                 AΤ
                      62
NSPEC
        IS C
                  AΤ
                      63
NSPEC
        IS C
                  ΑT
NSPEC
        IS C
                  AΤ
                      65
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
                       7 8 9 10 12 13 14 22 23 25 27 28 29 30 33 34 35
          36 37 38 39 44 45 46 47 48 49 54 55 56 57 59 60 61 62 64 66 67
          68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88
          89 90 91 92 93 94 95
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 95
STEREO ATTRIBUTES: NONE
=> s 1100
SAMPLE SEARCH INITIATED 22:42:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 806 TO ITERATE
100.0% PROCESSED
                     806 ITERATIONS
                                                               0 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                                **COMPLETE**
                       BATCH
```

14417 TO 17823

0 TO

h ebc gcg b

PROJECTED ITERATIONS:

PROJECTED ANSWERS:

NSPEC

IS C

AT 32

L101

0 SEA SSS SAM L100

=> s 1100 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: Y
FULL SEARCH INITIATED 22:42:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 16732 TO ITERATE

100.0% PROCESSED 16732 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L102

0 SEA SSS FUL L100

=>

```
C:\stnweb\queries\4.str
```

```
chain nodes :
    7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 43

ring nodes :
    1 2 3 4 5 6 25 26 27 28 29 30

chain bonds :
    6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23 23-24 23-31 24-26 31-32 31-33

ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

exact/norm bonds :
    8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 31-32 31-33

exact bonds :
    6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26

normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

isolated ring systems :
    containing 1 : 25 :
```

G1:0,S

G2:CH3,Et

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS

```
chain nodes :
```

```
7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42 ring nodes:
1 2 3 4 5 6 25 26 27 28 29 30 chain bonds:
6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23 23-24 23-31 24-26 28-42 29-41 31-32 31-33 ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30 exact/norm bonds:
8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 28-42 29-41 31-32 31-33 exact bonds:
6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30 solated ring systems:
containing 1: 25:
```

G2:CH3,Et

G1:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS
32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS

```
stnweb\Queries\9.str
```

```
ain nodes:
    7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42

ng nodes:
    1 2 3 4 5 6 25 26 27 28 29 30

ain bonds:
    6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23
    23-24 23-31 24-26 29-41 31-32 31-33

ng bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

act/norm bonds:
    8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 29-41 31-32 31-33

act bonds:
    6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26

rmalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30

olated ring systems:
    containing 1: 25:
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

:0,S

:CH3,Et

tch level :

```
C:\stnweb\Queries\9.str
```

```
chain nodes :
   7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42
ring nodes :
   1 2 3 4 5 6 25 26 27 28 29 30
chain bonds :
   6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23 23-24 23-31 24-26 28-42 31-32 31-33
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30
exact/norm bonds :
   8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 28-42 31-32 31-33
exact bonds :
   6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30
isolated ring systems :
   containing 1: 25:
G1:0,S
```

G2:CH3,Et

Match level:
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS

```
C:\stnweb\Queries\9a.str
```

```
7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42 ring nodes:
1 2 3 4 5 6 25 26 27 28 29 30 chain bonds:
6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23 23-24 23-31 24-26 28-42 30-41 31-32 31-33 ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30 exact/norm bonds:
8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 28-42 30-41 31-32 31-33 exact bonds:
6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30 isolated ring systems:
containing 1: 25:
```

G1:0,S

G2:CH3,Et

chain nodes :

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS

```
C:\stnweb\Queries\4.str
```

```
7 8 9 10 12 13 14 15 16 18 19 21 22 23 24 31 32 33 39 41 42 ring nodes:
1 2 3 4 5 6 25 26 27 28 29 30 chain bonds:
6-7 7-8 8-9 8-10 10-12 10-13 13-14 14-15 14-16 15-21 15-22 16-19 16-18 22-23 23-24 23-31 24-26 27-41 28-42 31-32 31-33 ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30 exact/norm bonds:
8-9 10-12 10-13 13-14 15-21 15-22 16-19 16-18 22-23 27-41 28-42 31-32 31-33 exact bonds:
6-7 7-8 8-10 14-15 14-16 23-24 23-31 24-26 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30 isolated ring systems: containing 1: 25:
```

G1:0,S

G2:CH3,Et

chain nodes :

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS

Welcome to STN International NEWS Web Page URLs for STN Seminar Schedule - N. America NEWS 2 "Ask CAS" for self-help around the clock NEWS May 12 EXTEND option available in structure searching May 12 Polymer links for the POLYLINK command completed in REGISTRY NEWS NEWS May 27 New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus CAplus super roles and document types searchable in REGISTRY NEWS 6 May 27 7 NEWS Jun 28 Additional enzyme-catalyzed reactions added to CASREACT ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, NEWS 8 Jun 28 and WATER from CSA now available on STN(R) Jul 12 BEILSTEIN enhanced with new display and select options, NEWS resulting in a closer connection to BABS NEWS 10 Jul 30 BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting NEWS 11 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields AUG 02 CAplus and CA patent records enhanced with European and Japan NEWS 12 Patent Office Classifications NEWS 13 AUG 02 STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting AUG 02 NEWS 14 The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available AUG 04 Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004 AUG 27 NEWS 16 BIOCOMMERCE: Changes and enhancements to content coverage NEWS 17 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC NEWS 18 SEP 01 INPADOC: New family current-awareness alert (SDI) available NEWS 19 SEP 01 New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! NEWS 20 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004 STN Operating Hours Plus Help Desk Availability NEWS HOURS NEWS INTER General Internet Information NEWS LOGIN Welcome Banner and News Items NEWS PHONE Direct Dial and Telecommunication Network Access to STN NEWS WWW CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004

cg

=> file reg
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
0.21
0.21

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2 DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See <u>HELP CROSSOVER</u> for details.

Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STI

=> s 1.1 ·

SAMPLE SEARCH INITIATED 21:04:20 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 21339 TO ITERATE

4.7% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

418042 TO 435518

PROJECTED ANSWERS:

149 TO 703

L2 1 SEA SSS SAM L1

=>

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STI

=> \$ 13

SAMPLE SEARCH INITIATED 21:05:37 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 11723 TO ITERATE

8.5% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 1 ANSWERS

1 ANSWERS

h ebc gcgb c

eb

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

> BATCH **COMPLETE**

PROJECTED ITERATIONS:

227975 TO 240945

PROJECTED ANSWERS:

29 TO 439

L4

L5

1 SEA SSS SAM L3

=> s 13 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 21:05:41 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 236139 TO ITERATE

100.0% PROCESSED 236139 ITERATIONS

128 ANSWERS

SEARCH TIME: 00.00.11

128 SEA SSS FUL L3

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TATOT

ENTRY

SESSION

FULL ESTIMATED COST

160.04

160.25

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLÉASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10 FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 15

L6

T.7

3 L5

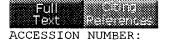
=> s 16 and matsuoka, h?/au

2095 MATSUOKA, H?/AU

1 L6 AND MATSUOKA, H?/AU

=> d 17, ibib abs fhitstr, 1

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN



2000:535162 HCAPLUS

DOCUMENT NUMBER:

133:150920

TITLE:

Preparation of peptides or analogs containing

substituted phenethylamine moiety as motilin receptor

antagonists

INVENTOR(S):

Matsuoka, Hiroharu; Sato, Tsutomu; Takahashi,

Tadakatsu; Kim, Dong Ick; Jung, Kyung Yun; Park, Chan

Нее

PATENT ASSIGNEE(S):

Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE:

GΙ

h

PCT Int. Appl., 403 pp. CODEN: PIXXD2

COI

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.					D	DATE			APPL	ICAT:	ION I	. OV		D	DATE 20000128 N, CR, CU, J, ID, IL, J, LV, MA, E, SG, SI, A, ZW, AM,			
	WO 2000044770			A1	_	2000	0803		wo 2	000-	JP44	4		2	0000	128			
	w:																		
		CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	ΗU,	ID,	IL,		
		IN,	IS,	JP,	ΚE,	KG,	KΡ,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,		
		MD,	MG,	MK,	MN,	MW,	MX,	NO,	ΝZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,		
		SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW,	AM,		
		ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	MT										
	RW:																		
		DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,		
		CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG						
	CA 2359	030			AΑ		2000	0803		CA 2	000-	<u> 2359</u>	030		2	0000	128		
																CR, CU, , ID, IL, , LV, MA, , SG, SI,			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	ΝL,	SE,	MC,	PT,		
		ΙE,	SI,	LT,	LV,	FI,	RO												
	NO 2001	.0036	84		A		2001	0928		<u>NO 2</u>	001-	<u> 3684</u>			2	0010	726		
PRIO	RITY APE	PLN.	INFO	.:					1	<u>JP 1</u>	999-	2052	<u>3</u>	i	A 1	9990	128		
							•			JP 1	999-	2831	<u>63</u>	i	A 1	9991	004		
										WO 2	000-	JP44	4	1	W 2	0000	128		
OTHE	R SOURCE	:(S):			MAR	PAT	133:	1509	20										

AB Substituted phenethylamine derivs. represented by general formula (I), hydrates of the same, or pharmaceutically acceptable salts thereof [wherein Cy is a group represented by general formula Q, an optionally substituted heterocyclic group, C3-7 cycloalkyl, or phenyl; R1, R1, R1, R1 and R5 are each hydrogen, halogeno, hydroxyl, amino, trifluoromethyl or cyano, at least one of R1-R5 being halogeno, trifluoromethyl or cyano; R6 represents hydrogen, (un)substituted linear or branched C1-3 alkyl, amino, or hydroxy; R8 represents hydrogen, Me, or ethyl; R9 represents (un)substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or C2-6 alkynyl, C3-7 cycloalkyl, or (un)substituted Ph; R20 represents hydrogen, or (un)substituted linear or branched C1-3 alkyl or R9 and R20 together forms C3-7 cycloalkyl; R10 represents hydrogen, (un)substituted linear or

branched C1-3 alkyl; R11 represents hydrogen or (un) substituted linear or branched C1-3 alkyl, (un) substituted carbamoyl, or carboxy; R12 represents hydroxy or linear or branched C1-4 alkoxy; R13 represents hydrogen, (un) substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or alkynyl, etc.; X, Y represents carbonyl or CH2; provisos are given.], which exhibit motilin receptor antagonism and being useful as drugs for preventing digestive tract movement or high level of blood motilin. Thus, 3-methyl-2-methylaminobutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2pyridylcarbamoyl)ethylamide (prepn. given) was condensed with Boc-Phe(4-F)-OH using CMPI in the presence of Et3N in THF under ice-cooling for 4 h followed by treatment of the product with CF3CO2H in CH2C12 gave 2-((2-amino-3-(4-fluorophenyl)propanoyl)-N-methylamino)-3methylbutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2pyridylcarbamoyl)ethylamide (II). II and N-Et-Phe(4-F)-N-Me-Val-N-Et-Tyr(3-tBu)-NHEt showed IC50 of 0.35 and 0.17 nM, resp., for inhibiting binding of 1251-motilin to motilin receptor prepn. from mucus membrane of rabbit duodenum.

IT 287205-81-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides or analogs contg. substituted phenethylamine moiety as motilin receptor antagonists and drugs for preventing digestive tract movement or high level of blood motilin)

RN <u>287205-81-6</u> HCAPLUS

CN L-Tyrosinamide, 4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N α -methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

L1

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004
STRUCTURE UPLOADED

L2 1 S L1

L3 STRUCTURE UPLOADED

L4 1 S L3

L5 128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5

L7 1 S L6 AND MATSUOKA, `H?/AU

```
=> s 16 not 17
```

L8 2 L6 NOT L7

=> s 18 and sato, t?/au

20671 SATO, T?/AU

L9 1 L8 AND SATO, T?/AU

=> d 19, ibib abs fhitstr, 1

L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Selgmannes

ACCESSION NUMBER:

2002:90066 HCAPLUS

DOCUMENT NUMBER:

136:135034

TITLE:

Method for producing tripeptide derivative

INVENTOR(S): Sato, Tsutomu; Shimizu, Hirohito

PATENT ASSIGNEE(S):

Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE:

PCT Int. Appl., 50 pp.

•

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	PATENT NO.					DATE		i	APPL	I CAT	ION 1	.00		D	TE 0010719 CH, CN, GE, GH, LK, LR,			
					_													
WO 2002	WO 2002008248			A1		2002	0131	1	WO 2	001-	JP62	<u>95</u>		20010719				
W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,		
	LS,	LT,	LU.	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	PL,	PT,		
	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	ΤZ,	UA,	UG,	US,		
	UΖ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM				
RW:	GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,		
	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	ΝL,	PT,	SE,	TR,	BF,		
	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML ,	MR,	NE,	SN,	TD,	TG			
PRIORITY APP	LN.	INFO	.:						JP 2	000-	2199	<u>77</u>	7	A 2	0000	721		
OTHER SOURCE(S):					REAC	Т 13	6:13	5034	; MA	RPAT	136	:135	034					
GI																		

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- Amethod for producing L-phenylalanyl-L-valyl-L-3-tert-butyl-L-tyrosinamide compds. represented by the general formula (I; wherein R1 represents a hydrogen atom or a linear or branched aliph. alkyl group having 1 to 4 carbon atoms; R2 represents a hydrogen atom or Me group; R3 represents a hydrogen atom or Me group; and R4 represents a halogen atom) comprises condensation of 3-tert-butyl-L-tyrosinamide derivs. (II; R1, R2 = same as above) with N-methyl-L-valine derivs. (III; P1 = amino-protecting group), N-deprotection of the resulting L-valyl-3-tert-butyl-L-tyrosinamide derivs. (IV; R1, R2, P1 = same as above), and condensation of the resulting IV (P1 = H; R1, R2 = same as above) with L-phenylalanine derivs. (V; R3, R4 = same as above; P2 = amino-protecting group) followed by N-deprotection. The method can be advantageously used for producing a novel peptide deriv. in a com. process. Thus, 20.8 g MeSO3H and 20.0 g tert-Bu chloride were

successively added to 10.0 g L-tyrosine Me ester hydrochloride under stirring, stirred at 50° for 5 h, treated dropwise with MeOH (20 mL)/H2O (20 mL) under ice-cooling then with a soln. of $14.2\,$ g KOH in $43\,$ mL $\mbox{H2O}$ at <10° to give 77.0% 3-tert-butyl-L-tyrosine Me ester which (8.35 g) was added to a mixt. of 24.1 g 62% aq. ethylamine and 7.52 gethylamine hydrochloride under ice-cooling and stirred at room temp. for 5 h to give 89.8% 3-tert-butyl-L-tyrosine ethylamide (VI). To a soln. of 5.50 g VI and 3.35 g 1-hydroxybenzotriazole monohydrate in 55 mL THF were successively added 4.19 g 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and 3.04 mL Et3N and stirred at room temp. for 2.5 h to give 100% N-tert-butoxycarbonyl-N-methyl-L-valyl-3-tert-butyl-L-tyrosine ethylamide which (10.0 g) was dissolved in 100 mL EtOAc, treated with 11.1 mL concd. H2SO4 under ice-cooling, treated with 100 mL EtOAc, adjusted pH 8 by adding satd. aq. NaHCO3, and stirred 15 min to give 87.9% N-methyl-L-valyl-3-tert-butyl-L-tyrosine ethylamide (VII). To a mixt. of 5.50 g VII, 5.20 g N-tert-butoxycarbonyl-N-methyl-4-fluoro-Lphenylalanine, 4.47 g 2-chloro-1-methylpyridinium iodide, and 37 mL tert-Bu Me ether was added $5.09~\mathrm{mL}$ Et3N and stirred at room temp. for $4~\mathrm{h}$ to give 86.0% N-tert-butoxycarbonyl-N-methyl-4-fluoro-L-phenylalanyl-Nmethyl-L-valyl-3-tert-butyl-L-tyrosine ethylamide which (7.50 g) was similarly deprotected as described above using concd. H2SO4 in EtOAc to give 100% N-methyl-4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-tert-butyl-Ltyrosine.

IT 393562-03-3P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. tripeptide derivs. by sequential coupling of N-methyl-L-valine derivs. and L-phenylalanine derivs. to 3-tert-butyl-L-tyrosinamide derivs.)

RN 393562-03-3 HCAPLUS

CN L-Tyrosinamide, N-[(1,1-dimethylethoxy)carbonyl]-4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N α -methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

7

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004 STRUCTURE UPLOADED

T.1

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L2
              1 S L1
L3
                STRUCTURE UPLOADED
T.4
              1 S L3
L5
            128 S L3 FULL
     FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004
              3 S L5
L6
Ļ7
              1 S L6 AND MATSUOKA, H?/AU
L8
              2 S L6 NOT L7
              1 S L8 AND SATO, T?/AU
1.9
=> s 18 not 19
            1 L8 NOT L9
L10
=> s 110 and takahashi, t?/au
         17491 TAKAHASHI, T?/AU
             0 L10 AND TAKAHASHI, T?/AU
T.11
=> s 110 and kim, d?/au
         13514 KIM, D?/AU
L12
            1 L10 AND KIM, D?/AU
=> d 12, ibib abs fhitstr, 1
      1 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):0
NUMBERS IN RANGE MUST BE GREATER THAN ZERO.
An answer number must be a positive number.
ENTER ANSWER NUMBER OR RANGE (1):0
NUMBERS IN RANGE MUST BE GREATER THAN ZERO.
An answer number must be a positive number.
ENTER ANSWER NUMBER OR RANGE (1):1
L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
         FULL
   Text
ACCESSION NUMBER:
                         2002:637704 HCAPLUS
DOCUMENT NUMBER:
                         137:185838
TITLE:
                         Process for preparation of peptide derivatives
```

INVENTOR(S): Kim, Dong Ick; Jeon, Gee Ho; Kim, Sung Jin

PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIN	D	DATE		1	APPLICATION NO.						DATE			
					-														
WO 2002064623				A1		2002	0822	,	WO 2	002-	JP11	<u>39</u> '		2	0020	212			
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
		GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,		
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	ΝZ,	OM,	PH,		
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	ΤZ,		
		UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,	KΖ,	MD,	RU,		
		ТJ,	TM																
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							FR,												

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO:

OTHER SOURCE(S):

CASREACT 137:185838; MARPAT 137:185838

GI

AB The title compds. I [Rl is hydrogen or linear or branched C1-4 alkyl; R2 is hydrogen or linear or branched C1-4 alkyl; and R3 is halogeno] are prepd. in a multistep process. I are motilin receptor antagonists and are useful as drugs for gastric or intestinal diseases (no data). Thus, amidation of N-(tert-butoxycarbonyl)-L-(4-fluorophenyl)alanine with L-valine Me ester hydrochloride, followed by methylation with iodomethane, sapon., reaction with 3-tert-butyl-L-tyrosine Et amide, and deprotection, gave N-methyl-L-4-fluorophenylalanyl-N-methyl-L-valine-3-tert-butyl-L-tyrosine Et amide.

Ι

IT 287206-61-5P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(process for prepn. of peptide derivs.)

RN <u>287206-61-5</u> HCAPLUS

CN L-Tyrosinamide, 4-fluoro-N-methyl-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004
L1 STRUCTURE UPLOADED

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1 S L1
L3
                STRUCTURE UPLOADED
              1 S L3
L4
            128 S L3 FULL
L5
     FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004
              3 S L5
L6
              1 S L6 AND MATSUOKA, H?/AU
L7
              2 S L6 NOT L7
Г8
              1 S L8 AND SATO, T?/AU
Ь9
L10
              1 S L8 NOT L9
L11
              0 S L10 AND TAKAHASHI, T?/AU
              1 S L10 AND KIM, D?/AU
L12
```

=> d 112, ibib abs fhitstr, 1

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

(B) (1) (P) Full Text

2002:637704 HCAPLUS ACCESSION NUMBER:

137:185838 DOCUMENT NUMBER:

Process for preparation of peptide derivatives TITLE:

Kim, Dong Ick; Jeon, Gee Ho; Kim, Sung Jin INVENTOR(S): Chugai Seiyaku Kabushiki Kaisha, Japan

PATENT ASSIGNEE(S): PCT Int. Appl., 40 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATEI	PATENT NO.						KIND DATE APPLICATION NO.							DATE			
WO 20	WO 2002064623				A1		2002	0822	3	wo 2	002-	JP11	<u> 39</u>		2	0020	212
Ţ	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,
		ТJ,	TM														
I	RW:	GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,
		CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	ĢW,	ML,	MR,	NE,	SN,	TD,	ΤG
PRIORITY A	PRIORITY APPLN. INFO.:									KR 2	001-	6673			A 2	0010	212
OTHER SOU	OTHER SOURCE(S):					CASREACT 137:185838; MARPAT 137:185838											
GI																	

The title compds. I [R1 is hydrogen or linear or branched C1-4 alkyl; R2 is hydrogen or linear or branched C1-4 alkyl; and R3 is halogeno] are prepd. in a multistep process. I are motilin receptor antagonists and are useful as drugs for gastric or intestinal diseases (no data). Thus, amidation of N-(tert-butoxycarbonyl)-L-(4-fluorophenyl)alanine with L-valine Me ester hydrochloride, followed by methylation with iodomethane, sapon., reaction with 3-tert-butyl-L-tyrosine Et amide, and deprotection, gave N-methyl-L-4-fluorophenylalanyl-N-methyl-L-valine-3-tert-butyl-L-tyrosine Et amide.

I

IT 287206-61-5P

CN

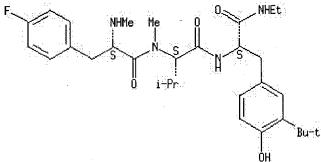
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(process for prepn. of peptide derivs.)

RN <u>287206-61-5</u> HCAPLUS

L-Tyrosinamide, 4-fluoro-N-methyl-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

SINCE FILE	TOTAL
ENTRY	SESSION
28.48	188.73
SINCE FILE	TOTAL
ENTRY	SESSION
-2.80	-2.80
	ENTRY 28.48 SINCE FILE ENTRY

FILE 'CAOLD' ENTERED AT 21:08:12 ON 02 SEP 2004
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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter <u>HELP FIRST</u> for more information.

=> d his

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004

L1 STRUCTURE UPLOADED L2 1 S L1

L3 STRUCTURE UPLOADED

L4 1 S L3 L5 128 S L3

128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5

L7 1 S L6 AND MATSUOKA, H?/AU

L8 2 S L6 NOT L7

L9 1 S L8 AND SATO, T?/AU

L10 1 S L8 NOT L9

L11 0 S L10 AND TAKAHASHI, T?/AU

L12 1 S L10 AND KIM, D?/AU

FILE 'CAOLD' ENTERED AT 21:08:12 ON 02 SEP 2004

=> s 15

L13 0 L5

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 0.42 189.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

CA SUBSCRIBER PRICE ENTRY SESSION 0.00 -2.80

FILE 'REGISTRY' ENTERED AT 21:08:18 ON 02 SEP 2004
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Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by ${\tt InfoChem.}$

STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2 DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See <u>HELP CROSSOVER</u> for details.

Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>

L14 STRUCTURE UPLOADED

=> d 114

L14 HAS NO ANSWERS L14 STR

=> s 114 SAMPLE SEARCH INITIATED 21:09:07 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 11723 TO ITERATE

8.5% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

227975 TO 240945

PROJECTED ANSWERS:

29 TO 43

L15 1 SEA SSS SAM L14

=> s 114 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: Y
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FULL SCREEN SEARCH COMPLETED - 236139 TO ITERATE

100.0% PROCESSED 236139 ITERATIONS SEARCH TIME: 00.00.12

128 ANSWERS

DEFINION TIME. 00:00:12

L16 128 SEA SSS FUL L14

=> d his

(FILE 'HOME' ENTERED AT 20:58:31 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 20:58:58 ON 02 SEP 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 STRUCTURE UPLOADED

L4 1 S L3

L5 128 S L3 FULL

FILE 'HCAPLUS' ENTERED AT 21:05:55 ON 02 SEP 2004

L6 3 S L5

L7 1 S L6 AND MATSUOKA, H?/AU

L8 2 S L6 NOT L7

L9 1 S L8 AND SATO, T?/AU

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1 S L8 NOT L9
           0 S L10 AND TAKAHASHI, T?/AU
L11
           1 S L10 AND KIM, D?/AU
L12
    FILE 'CAOLD' ENTERED AT 21:08:12 ON 02 SEP 2004
L13
      0 S L5
   FILE 'REGISTRY' ENTERED AT 21:08:18 ON 02 SEP 2004
L14
       STRUCTURE UPLOADED
           1 S L14
L15
L16
          128 S L14 FULL
=> s 116 not 15
L17 0 L16 NOT L5
=>
L18 STRUCTURE UPLOADED
=> d 118
L18 HAS NO ANSWERS
L18
             STR
811 a <=
SAMPLE SEARCH INITIATED 21:10:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21339 TO ITERATE
 4.7% PROCESSED 1000 ITERATIONS
                                                          1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS: 418042 TO 435518
PROJECTED ANSWERS:
                           149 TO 703
           1 SEA SSS SAM L18
L19
=>
L20
     STRUCTURE UPLOADED
=> d 1.20
L20 HAS NO ANSWERS
L20
=> s 120
SAMPLE SEARCH INITIATED 21:11:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21339 TO ITERATE
 4.7% PROCESSED
                 1000 ITERATIONS
                                                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS:
                      418042 TO 435518
                             0 TO
PROJECTED ANSWERS:
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h ebc gcg b cg

0 SEA SSS SAM L20

L21

L22 STRUCTURE UPLOADED

=> d 122

L22 HAS NO ANSWERS

=> s 122

SAMPLE SEARCH INITIATED 21:12:17 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 153 TO ITERATE

100.0% PROCESSED 153 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

2318 TO

PROJECTED ANSWERS:

O TO

L23

0 SEA SSS SAM L22

=> s 122

SAMPLE SEARCH INITIATED 21:12:20 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 153 TO ITERATE

100.0% PROCESSED 153 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

2318 TO 3802

PROJECTED ANSWERS:

O TO

L24

0 SEA SSS SAM L22

=> s 122 full

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100.0% PROCESSED 2746 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L25 0 SEA SSS FUL L22

=>

STRUCTURE UPLOADED L26

=> 126

L26 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter ""HELP COMMANDS" at an arrow prompt (=>).

=> d 126

L26 HAS NO ANSWERS

L26

STR

=> s 126

SAMPLE SEARCH INITIATED 21:13:07 FILE 'REGISTRY'

h eb c g cg b SAMPLE SCREEN SEARCH COMPLETED - 342 TO ITERATE

100.0% PROCESSED 342 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

5731 TO 7949

PROJECTED ANSWERS:

0 TO

L27

0 SEA SSS SAM L26

=> s 126 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 21:13:12 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 7164 TO ITERATE

100.0% PROCESSED 7164 ITERATIONS

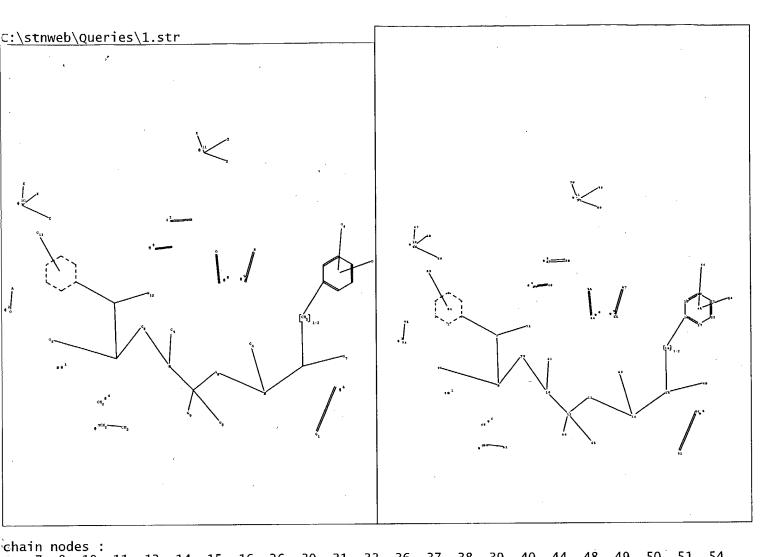
0 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.01

L28 0 SEA SSS FUL L26

=>



7 8 10 11 12 14 15 16 26 30 31 33 36 37 38 39 40 44 48 49 50 51 54 55 56 57 61 62 64 65 66 67 68 69 72 73 74 75 77 78 79 80 83 ring nodes:
1 2 3 4 5 6 17 18 19 20 21 22 chain bonds:
6-7 7-8 7-72 8-36 8-73 10-61 10-11 10-73 11-12 11-64 11-65 12-14 14-15 14-62 15-16 15-48 16-18 30-31 37-38 39-40 50-51 54-55 56-57 66-68 66-69 66-67 74-75 77-79 77-80 77-78 ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22 exact/norm bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-72 8-36 10-61 10-11 11-12 11-64 11-65 12-14 14-15 14-62 15-48 30-31 54-55 56-57 74-75 exact bonds:
6-7 7-8 8-73 10-73 15-16 16-18 37-38 39-40 50-51 66-68 66-69 66-67 77-79 77-80 77-78 normalized bonds:
17-18 17-22 18-19 19-20 20-21 21-22 isolated ring systems:
containing 1: 17:

G1:0,S

G2:CH3,Et

G3:H,Ak

G4:CH3,Et,H

G5:Ak,H,OH,[*1],[*2]

G6:Ak,Cb,[*3],[*4]

```
G7:COOH,Ak,H,[*5]
```

G8: [*6], [*7], [*8], [*9]

G9:Ak,Ph

G12:H,OH,NH2,CN,[*10]

G13:CN,X,[*11]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 31:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CL 12:CLASS 14:CLASS 15:CLASS 16:CLASS 22:Atom 26:CLASS 27:CLASS 30:CLASS 31:CLASS 38:CLASS 44:CLASS 57:CLASS 51:CLASS 54:CLASS 45:CLASS 48:CLASS 49:CLASS 50:CLASS 39:CLASS 40:CLASS 66:CLASS 67:CLASS 56:CLASS 61:CLASS 62:CLASS 64:CLASS 65:CLASS 55:CLASS 72:CLASS 75:CLASS 77:CLASS 78:CLASS 79:CLASS 73:CLASS 74:CLASS 68:CLASS 69:CLASS 83:CLASS 80:CLASS 84:CLASS

=>

STRUCTURE UPLOADED L124

=> d 1124

L124 HAS NO ANSWERS

L124

=> s 1124

SAMPLE SEARCH INITIATED 23:29:57 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 17092 TO ITERATE

5.9% PROCESSED 1000 ITERATIONS 1 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 334015 TO 349665

PROJECTED ANSWERS:

93 TO 589

L125

1 SEA SSS SAM L124

=> s 1125

SAMPLE SEARCH INITIATED 23:30:08 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 17092 TO ITERATE

1000 ITERATIONS 5.9% PROCESSED

1 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 334015 TO 349665

PROJECTED ANSWERS:

93 TO 589

L126

1 SEA SSS SAM L124

=> s 1125 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END: Y

FULL SEARCH INITIATED 23:30:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 342655 TO ITERATE

100.0% PROCESSED 342655 ITERATIONS

353 ANSWERS

SEARCH TIME: 00.00.16

L127

h

353 SEA SSS FUL L124

=> file hcaplus

SINCE FILE TOTAL COST IN U.S. DOLLARS

ENTRY SESSION

FULL ESTIMATED COST 329.32 3308,11

SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SESSION ENTRY 0.00 -9.10 CA SUBSCRIBER PRICE

FILE 'HCAPLUS' ENTERED AT 23:31:50 ON 02 SEP 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

eb

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FILE COVERS 1907 - 2 Sep 2004 VOL 141 ISS 10 FILE LAST UPDATED: 1 Sep 2004 (20040901/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 1127 °

L128

4 L127

=> s 1128 and matsuoka, ha/au

2095 MATSUOKA, H?/AU

2095 MAISOOKA, II:/A0

L129 2 L128 AND MATSUOKA, H?/AU

=> d 129, ibib abs fhitstr, 1-2

L29 HAS NO ANSWERS

'IBIB ABS FHITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ---- Structure Image, Attributes, and map table if it contains

data. (Default)

SIM ---- Structure IMage.

SAT ---- Structure ATtributes and map table if it contains data.

SCT ---- Structure Connection Table and map table if it contains

data.

SDA ---- All Structure DAta (image, attributes, connection table and

map table if it contains data).

NOS ---- NO Structure data.

ENTER STRUCTURE FORMAT (SIA), SCT, SDA, SIM, SAT, NOS: end

=> d 1129, ibib abs fhitstr, 1-2

L129 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

FUL Text

ACCESSION NUMBER: 2002:157810 HCAPLUS

DOCUMENT NUMBER: 136:217049

TITLE: Preparation of cyclic peptide derivatives as motilin

receptor antagonists

INVENTOR(S): Matsuoka, Hiroharu; Sato, Tsutomu

PATENT ASSIGNEE(S): Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE: PCT Int. Appl., 89 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	rent :	ΝΟ.			KIN		DATE			APPL						ATE	
WO	2002	0164	04														
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GΜ,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	ΜK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PH,	PL,
		PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	ŪG,
		US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	$\mathbf{T}\mathbf{M}$	
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZW,	ΑT,	BE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
AU								AU 2001-80120									
EP	EP 1312612				A1 20030521			EP 2001-958426				20010823					
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	ΜK,	CY,	AL,	TR						
US	2003	1910	53		A1		2003	1009		US 2	003-	3625	74		2	0030	224
PRIORITY	PRIORITY APPLN. INFO.:			.:						JP 2	000-	2539	50		A 2	0000	824
										WO 2	001-	JP72	13	1	₩ 2	0010	823
OTHER SO	OURCE	(S):			MAR	PAT	136:	2170	49				•				

GΙ

RN

AB The title compds. I [T1 = (CH2)m; T2 = (CH2)n; R1 represents optionally substituted Ph, etc.; R2 represents amino, etc.; R3 to R6 each represents hydrogen, Me, etc.; V, W, X,Y, Z represent carbonyl or methylene; m is an integer of 0 to 2; and n is an integer of 0 to 3] are prepd. In an in vitro test for motilin receptor antagonism, (2S-(2S,12S))-2-amino-N-(2-(3-tert-butyl-4-hydroxylphenylmethyl)-1,4,8-triaza-3,7,13-trioxocyclotridecan-12-yl)-3-(4-fluorophenyl)-N-methylpropionamide showed IC50 of 0.52 nM.

IT 401896-13-7P

I

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cyclic peptide derivs. as motilin receptor antagonists) 401896-13-7 HCAPLUS

CN β -Alanine, N-[(1,1-dimethylethoxy)carbonyl]-4-fluoro-L-phenylalanyl-N2-methyl-N6-[(phenylmethoxy)carbonyl]-L-lysyl-3-(1,1-dimethylethyl)-L-tyrosyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2004 ACS on STN L129 ANSWER 2 OF 2

Text

ACCESSION NUMBER:

2000:535162 HCAPLUS

DOCUMENT NUMBER:

133:150920

TITLE:

Preparation of peptides or analogs containing

substituted phenethylamine moiety as motilin receptor

antagonists

INVENTOR(S):

Matsuoka, Hiroharu; Sato, Tsutomu; Takahashi,

Tadakatsu; Kim, Dong Ick; Jung, Kyung Yun; Park, Chan

PATENT ASSIGNEE(S):

Chugai Seiyaku Kabushiki Kaisha, Japan

SOURCE:

PCT Int. Appl., 403 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO		KIND	DATE	APPLICATION NO.	DATE			
WO 200004	<u>4770</u>	A1	20000803	WO 2000-JP444	20000128			
W: Al	E, AL, A	M, AT, A	U, AZ, BA,	BB, BG, BR, BY, CA,	CH, CN, CR, CU,			
C	Z, DE, D	K, DM, E	E, ES, FI,	GB, GD, GE, GH, GM,	HR, HU, ID, IL,			
· II	N, IS, J	P, KE, K	G, KP, KR,	KZ, LC, LK, LR, LS,	LT, LU, LV, MA,			
M	D, MG, M	K, MN, M	W, MX, NO,	NZ, PL, PT, RO, RU,	SD, SE, SG, SI,			
SI	K, SL, T	J, TM, T	R, TT, TZ,	UA, UG, US, UZ, VN,	YU, ZA, ZW, AM,			
A	Z, BY, K	G, KZ, M	D, RU, TJ,	TM	•			
RW: G	н, GM, К	E, LS, M	W, SD, SL,	SZ, TZ, UG, ZW, AT,	BE, CH, CY, DE,			
Di	K, ES, F	I, FR, G	B, GR, IE,	IT, LU, MC, NL, PT,	SE, BF, BJ, CF,			
C	G, CI, C	M, GA, GI	N, GW, ML,	MR, NE, SN, TD, TG				
CA 235903	CA 2359030			CA 2000-2359030	20000128			
EP 114984	EP 1149843			EP 2000-901956	20000128			
R: A	т, ве, с	H, DE, DI	K, ES, FR,	GB, GR, IT, LI, LU,	NL, SE, MC, PT,			
I	E, SI, L	r, LV, F	I, RO					
NO 200100	NO 2001003684			NO 2001-3684	20010726			
PRIORITY APPLN	RIORITY APPLN. INFO.:			JP 1999-20523	A 19990128			
				JP 1999-283163	A 19991004			
				WO 2000-JP444	W 20000128			
OTHER SOURCE (S	OTHER SOURCE (S):			20				

GΙ

Substituted phenethylamine derivs. represented by general formula (I), AB hydrates of the same, or pharmaceutically acceptable salts thereof [wherein Cy is a group represented by general formula Q, an optionally substituted heterocyclic group, C3-7 cycloalkyl, or phenyl; R1, R1, R1, R1 and R5 are each hydrogen, halogeno, hydroxyl, amino, trifluoromethyl or cyano, at least one of R1-R5 being halogeno, trifluoromethyl or cyano; R6 represents hydrogen, (un) substituted linear or branched C1-3 alkyl, amino, or hydroxy; R8 represents hydrogen, Me, or ethyl; R9 represents (un) substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or C2-6 alkynyl, C3-7 cycloalkyl, or (un) substituted Ph; R20 represents hydrogen, or (un) substituted linear or branched C1-3 alkyl or R9 and R20 together forms C3-7 cycloalkyl; R10 represents hydrogen, (un) substituted linear or branched C1-3 alkyl; R11 represents hydrogen or (un) substituted linear or branched C1-3 alkyl, (un) substituted carbamoyl, or carboxy; R12 represents hydroxy or linear or branched C1-4 alkoxy; R13 represents hydrogen, (un) substituted linear or branched C1-6 alkyl, C2-6 alkenyl, or alkynyl, etc.; X, Y represents carbonyl or CH2; provisos are given.], which exhibit motilin receptor antagonism and being useful as drugs for preventing digestive tract movement or high level of blood motilin. Thus, 3-methyl-2-methylaminobutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2pyridylcarbamoyl)ethylamide (prepn. given) was condensed with Boc-Phe(4-F)-OH using CMPI in the presence of Et3N in THF under ice-cooling for 4 h followed by treatment of the product with CF3CO2H in CH2C12 gave 2-((2-amino-3-(4-fluorophenyl)propanoyl)-N-methylamino)-3methylbutyric acid 2-(3-tert-butyl-4-hydroxyphenyl)-1-(2pyridylcarbamoyl)ethylamide (II). II and N-Et-Phe(4-F)-N-Me-Val-N-Et-Tyr(3-tBu)-NHEt showed IC50 of 0.35 and 0.17 nM, resp., for inhibiting binding of 125I-motilin to motilin receptor prepn. from mucus membrane of rabbit duodenum.

IT 287205-81-6P

RN

h

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptides or analogs contg. substituted phenethylamine moiety as motilin receptor antagonists and drugs for preventing digestive tract movement or high level of blood motilin)

287205-81-6 HCAPLUS

CN L-Tyrosinamide, 4-fluoro-L-phenylalanyl-N-methyl-L-valyl-3-(1,1-dimethylethyl)-N\alpha-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION 61.44 3369.55 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -10.50CA SUBSCRIBER PRICE -1.40

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter <u>HELP FIRST</u> for more information.

=> d his

h

(FILE 'HOME' ENTERED AT 21:22:36 ON 02 SEP 2004)

FILE 'REGISTRY' ENTERED AT 21:22:42 ON 02 SEP 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 196 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 21:26:58 ON 02 SEP 2004
L4 STRUCTURE UPLOADED
S L4

FILE 'REGISTRY' ENTERED AT 21:28:05 ON 02 SEP 2004 L5 1 S L4

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FILE 'HCAPLUS' ENTERED AT 21:28:06 ON 02 SEP 2004
L6
              1 S L5
     FILE 'REGISTRY' ENTERED AT 21:28:09 ON 02 SEP 2004
L7
                STRUCTURE UPLOADED
L8
              1 S L7
     FILE 'HCAPLUS' ENTERED AT 21:28:41 ON 02 SEP 2004
L9
              4 S L3
     FILE 'CAOLD' ENTERED AT 21:29:13 ON 02 SEP 2004
L10
              0 S L9
     FILE 'REGISTRY' ENTERED AT 21:29:19 ON 02 SEP 2004
L11
               STRUCTURE UPLOADED
L12
              2 S L11
L13
            352 S L11 FULL
     FILE 'HCAPLUS' ENTERED AT 21:31:02 ON 02 SEP 2004
              7 S L13
L14
L15
              3 S L14 NOT L9
L16
              1 S L15 AND MATSUOKA, H?/AU
L17
              2 S L15 NOT L16
L18
              1 S L17 AND SATO, T?/AU
L19
              1 S L17 NOT L18
L20
              0 S L19 AND TAKAHASHI, T?/AU
L21
              0 S L17 AND KIM, D?/AU
L22
              0 S L17 AND JUNG, K?/AU
L23
              0 S L17 AND PARK, C?/AU
              0 S L19 AND KIM, D?/AU
L25
              0 S L19 AND PARK, C?/AU
     FILE 'CAOLD' ENTERED AT 21:33:05 ON 02 SEP 2004
L26
              0 S L13
     FILE 'REGISTRY' ENTERED AT 21:33:13 ON 02 SEP 2004
L27
              STRUCTURE UPLOADED
L28
              2 S L27
L29
               STRUCTURE UPLOADED
L30
             50 S L29
L31
          15669 S L29 FULL
     FILE 'HCAPLUS' ENTERED AT 21:35:22 ON 02 SEP 2004
L32
         8855 S L31
     FILE 'REGISTRY' ENTERED AT 21:35:31 ON 02 SEP 2004
                STRUCTURE UPLOADED
L33
L34
             50 S L33
L35
                STRUCTURE UPLOADED
L36
             0 S L35
L37
            347 S L35 FULL
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L38
              7 S L37
L39
              0 S L38 NOT L14
     FILE 'REGISTRY' ENTERED AT 21:38:35 ON 02 SEP 2004
L40
               STRUCTURE UPLOADED
L41
              2 S L40
L42
            351 S L40 FULL
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              7 S L42
L43
     FILE 'REGISTRY' ENTERED AT 21:41:41 ON 02 SEP 2004
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L44
L45
             50 S L44
L46
               STRUCTURE UPLOADED
L47
              2 S L46
            351 S L46 FULL
L48
L49
                STRUCTURE UPLOADED
L50
              2 S L49
L51
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L52
              7 S L51
     FILE 'REGISTRY' ENTERED AT 21:47:42 ON 02 SEP 2004
L53
                STRUCTURE UPLOADED
L54
              2 S L53
L55
            439 S L53 FULL
     FILE 'HCAPLUS' ENTERED AT 21:50:36 ON 02 SEP 2004
L56
           10 S L55
              3 S L56 NOT L43
L57
     FILE 'CAOLD' ENTERED AT 21:52:39 ON 02 SEP 2004
              0 S L55
L58
     FILE 'REGISTRY' ENTERED AT 21:52:47 ON 02 SEP 2004
               STRUCTURE UPLOADED
L59
              2 S L59
L60
L61
            439 S L59 FULL
     FILE 'HCAPLUS' ENTERED AT 21:57:31 ON 02 SEP 2004
L62
            10 S L61
     FILE 'REGISTRY' ENTERED AT 21:57:38 ON 02 SEP 2004
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L63
L64
              2 S L63
L65
                STRUCTURE UPLOADED
                STRUCTURE UPLOADED
L66
              2 S L66
L67
L68
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L69
              1 S L68
L70
                STRUCTURE UPLOADED
L71
              0 S L70
L72
                STRUCTURE UPLOADED
L73
              0 S L72
L74
             10 S L72 FULL
L75
                STRUCTURE UPLOADED
L76
              0 S L75
L77
              0 S L74 NOT L61
L78
                STRUCTURE UPLOADED
L79
              0 S L78
L80
              0 S L78 FULL
L81
                STRUCTURE UPLOADED
L82
              0 S L81
L83
              0 S L81 FULL
                STRUCTURE UPLOADED
L84
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L86
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L87
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F88
             0 S L87 FULL
L89
L90
               STRUCTURE UPLOADED
L91
             0 S L90
L92
              STRUCTURE UPLOADED
L93
             0 S L92
           0 S L92 FULL
L94
L95
               STRUCTURE UPLOADED
L96
             0 S L95
L97
             5 S L95 FULL
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L98
             1 S L97
    FILE 'CAOLD' ENTERED AT 22:41:17 ON 02 SEP 2004
L99
             0 S L97
    FILE 'REGISTRY' ENTERED AT 22:41:28 ON 02 SEP 2004
L100
              STRUCTURE UPLOADED
L101
             0 S L100
L102
             0 S L100 FULL
L103
               STRUCTURE UPLOADED
L104
            1 S L103
L105
               STRUCTURE UPLOADED
L106
            0 S L105
               STRUCTURE UPLOADED
L107
L108
            0 S L107
L109
            41 S L107 FULL
    FILE 'HCAPLUS' ENTERED AT 22:56:53 ON 02 SEP 2004
             2 S L109
    FILE 'CAOLD' ENTERED AT 23:00:44 ON 02 SEP 2004
L111
             0 S L109
    FILE 'HCAPLUS' ENTERED AT 23:00:59 ON 02 SEP 2004
L112
           1 S 130:19658/DN
               SEL RN
    FILE 'HCAPLUS' ENTERED AT 23:01:37 ON 02 SEP 2004
L113 880326 S E1-E4
    FILE 'REGISTRY' ENTERED AT 23:02:05 ON 02 SEP 2004
             4 S E1-E4
L114
     FILE 'REGISTRY' ENTERED AT 23:02:44 ON 02 SEP 2004
    FILE 'HCAPLUS' ENTERED AT 23:03:10 ON 02 SEP 2004
L115
          1 S 130:196958/DN
               SEL RN
    FILE 'REGISTRY' ENTERED AT 23:03:32 ON 02 SEP 2004
    FILE 'HCAPLUS' ENTERED AT 23:03:38 ON 02 SEP 2004
               DELETE SELECT
               SEL RN
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L85

0 S L84

FILE 'REGISTRY' ENTERED AT 23:04:01 ON 02 SEP 2004 276 S E1-E276 L116 STRUCTURE UPLOADED L117 L118 0 S L117 0 S L118 FULL L119 L120 STRUCTURE UPLOADED L121 2 S L120 L122 STRUCTURE UPLOADED L123 2 S L122 STRUCTURE UPLOADED L124 L125 1 S L124 L126 1 S L125 L127 353 S L125 FULL FILE 'HCAPLUS' ENTERED AT 23:31:50 ON 02 SEP 2004 L128 4 S L127

FILE 'CAOLD' ENTERED AT 23:44:54 ON 02 SEP 2004

2 S L128 AND MATSUOKA, H?/AU

=> s 1127

L129

L130 0 L127

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	3369.97
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
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FILE 'REGISTRY' ENTERED AT 23:45:20 ON 02 SEP 2004
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STRUCTURE FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2 DICTIONARY FILE UPDATES: 1 SEP 2004 HIGHEST RN 737690-81-2

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

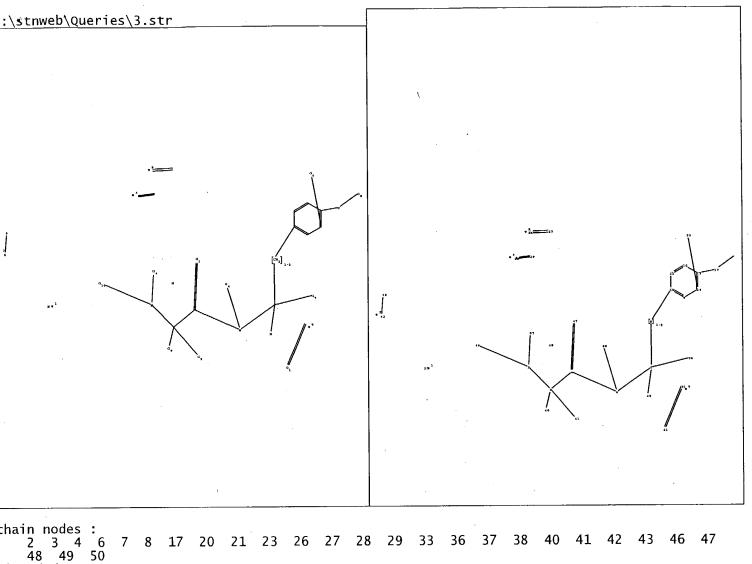
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See <u>HELP CROSSOVER</u> for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/online/DBSS/registryss.html

=>

h



```
48 49 50
ring nodes:
9 10 11 12 13 14
chain bonds:
2-37 2-3 2-46 3-4 3-40 3-41 4-6 4-47 6-7 6-38 7-8 7-36 7-49 8-10 13-17
14-33 17-50 20-21 26-27 28-29 42-43
ring bonds:
9-10 9-14 10-11 11-12 12-13 13-14
exact/norm bonds:
2-37 2-3 2-46 3-40 3-41 4-6 4-47 6-7 6-38 7-36 13-17 14-33 17-50 20-21
42-43
exact bonds:
3-4 7-8 7-49 8-10 26-27 28-29
normalized bonds:
9-10 9-14 10-11 11-12 12-13 13-14
```

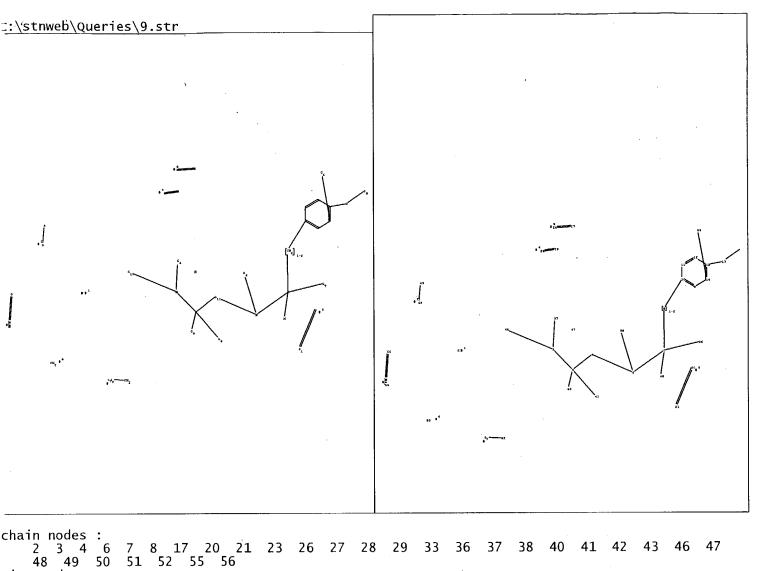
G2:CH3,Et G3:H,Ak G4:CH3,Et,H G5:Ak,H,OH,[*1],[*2] G6:Ak,Cb,[*3],[*4] G7:COOH,Ak,H,[*5]

51:0,S

G9:Ak,Ph

10:H,A

atch level:
2:CLASS 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 17:CLASS 20:CLASS 21:CLASS 23:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS



```
48 49 50 51 52 55 56
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9 10 11 12 13 14
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2-37 2-3 2-46 3-4 3-40 3-41 4-6 6-7 6-38 7-8 7-36 7-48 8-10 13-17 14-33 17-49 20-21 26-27 28-29 42-43 51-52 55-56
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3-4 7-8 7-48 8-10 26-27 28-29 51-52
normalized bonds:
9-10 9-14 10-11 11-12 12-13 13-14
```

G1:0,S G2:CH3,Et G3:H,Ak G4:CH3,Et,H

G5:Ak,H,OH,[*1],[*2]

G6:Ak,Cb,[*3],[*4]

G7:COOH,Ak,H,[*5]

G9:Ak,Ph

0:H,A

1:[*6],[*7],[*8]

tch level:

2:CLASS 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 17:CLASS 20:CLASS 21:CLASS 23:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 33:CLASS 36:CLASS 37:CLASS 38:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 55:CLASS 56:CLASS

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FILE 'HOME' ENTERED AT 14:13:41 ON 03 SEP 2004

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION FULL ESTIMATED COST 0.21 0.21

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STRUCTURE FILE UPDATES: 2 SEP 2004 HIGHEST RN 737922-52-0 2 SEP 2004 HIGHEST RN 737922-52-0 DICTIONARY FILE UPDATES:

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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=> L1STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS

 \Rightarrow s 11 SAMPLE SEARCH INITIATED 14:17:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 33736 TO ITERATE

3.0% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

> BATCH **INCOMPLETE**

PROJECTED ITERATIONS: 663752 TO 685688

PROJECTED ANSWERS: 857 TO

2 SEA SSS SAM L1

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 14:24:21 ON 03 SEP 2004 FILE 'REGISTRY' ENTERED AT 14:24:21 ON 03 SEP 2004 COPYRIGHT (C) 2004 American Chemical Society (ACS) COST IN U.S. DOLLARS SINCE FILE

ENTRY SESSION FULL ESTIMATED COST 7.14 7.35

=> L3 STRUCTURE UPLOADED

h eb c g cg b cg 2 ANSWERS

TOTAL

1 ANSWERS

0 ANSWERS

0 ANSWERS

=> d 13

L3 HAS NO ANSWERS

.3 ST

=> s 13

SAMPLE SEARCH INITIATED 14:26:28 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 29316 TO ITERATE

3.4% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 576090 TO 596550

PROJECTED ANSWERS: 262 TO 910

L4 1 SEA SSS SAM L3

=>

L5 STRUCTURE UPLOADED

=> d 3.5

L5 HAS NO ANSWERS

L5 STI

=> s 15

SAMPLE SEARCH INITIATED 14:27:45 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 29316 TO ITERATE

3.4% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 576090 TO 596550

PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=>

L7 STRUCTURE UPLOADED

=> s 17

SAMPLE SEARCH INITIATED 14:29:33 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 14078 TO ITERATE

7.1% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 274455 TO 288665

PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 full

h ebc gcgb cg

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: γ FULL SEARCH INITIATED 14:29:38 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 282169 TO ITERATE

100.0% PROCESSED 282169 ITERATIONS

0 ANSWERS

0 ANSWERS

SEARCH TIME: 00.00.13

L9

0 SEA SSS FUL L7

=>

I.10 STRUCTURE UPLOADED

=> d 110

L10 HAS NO ANSWERS

L10

STR

=> s 110

SAMPLE SEARCH INITIATED 14:32:06 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 15187 TO ITERATE

6.6% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

296362 TO 311118

PROJECTED ANSWERS:

0 TO

L11 0 SEA SSS SAM L10

=> s 110 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: $_{\Upsilon}$ FULL SEARCH INITIATED 14:32:11 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 303479 TO ITERATE

100.0% PROCESSED 303479 ITERATIONS

0 ANSWERS

323.23

SEARCH TIME: 00.00.14

L12

0 SEA SSS FUL L10

=> roa X

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 323.02

STN INTERNATIONAL LOGOFF AT 14:32:36 ON 03 SEP 2004